Numerical simulation of polyester coextrusion: Influence of the thermal parameters and the die geometry on interfacial instabilities

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Abstract. The polymer coextrusion process is a new method of sheet metal lining. It allows to substitute lacquers for steel protection in food packaging industry. The investigation shows that the coextrusion process exhibits some flow instability at the interface. The objective of this work is to test the influence of there processing and rheology parameters on the instabilities. Finite elements numerical simulations of the coextrusion are using to determine conditions to obtain a stable configuration.

Keywords: Coextrusion, interface instability, rheology, viscosity, elasticity, die

INTRODUCTION

This process consists in extruding different polymers in the same die in order to get a multi-layer product which will provide simultaneously adhesion properties (on metal) as well as mechanical and printing properties for the coating. In the given study, the film is composed of two layers. For some processing conditions, instabilities are observed at the layers interface in the die [1][2] (Figure 1). These instabilities involve unwanted heterogeneities.

Experimental and theoretical studies pointed out the effect of material properties, layer ratio and processing condition. There are few experimental studies concerning coextrusion instability for commercial polymers and complex die [2][3]. The experimental and numerical studies show that these instabilities depend on several parameters, e.g. processing temperature and flow rates, differences in viscosity and elasticity [4][5][6][7].

In this paper we show the role of the die design and rheology of coextruded materials from the interfacial instability point of view. Initially, we were interested in monolayer 3D computation and we investigated then 2D computation (isothermal and non isothermal models).

Geometry and materials

We consider the geometry of “coat hanger” flat die presented in Figure 2. The die is composed of three zones; the first region a low width and a high thickness feeder canal.

The die finishes in the third part which is wider and thinner. The second zone, called “coat hanger” connects previous zones.

Two kinds of polymer have been considered (PET1 and PET2). Dynamic rheology measurements were performed at different temperatures. Figure 3 shows the master curve of the viscosity and relaxation time obtained at 260°C, for PET1 and PET2. Two kinds of polymer have respectively a Newtonian and shear thinning rheological behaviour. To describe the behaviour of PET1 and PET2, we carried out an interpolation based on Carreau-Yasuda model to get viscosity and relaxation time curves.

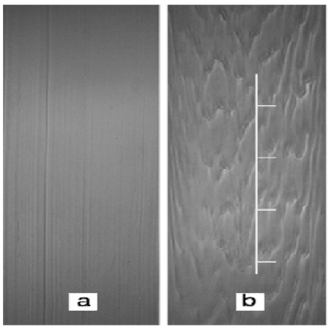


Figure 1: (a) stable, (b) instable

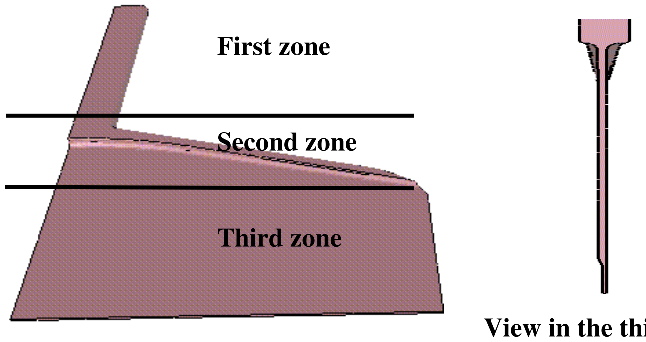
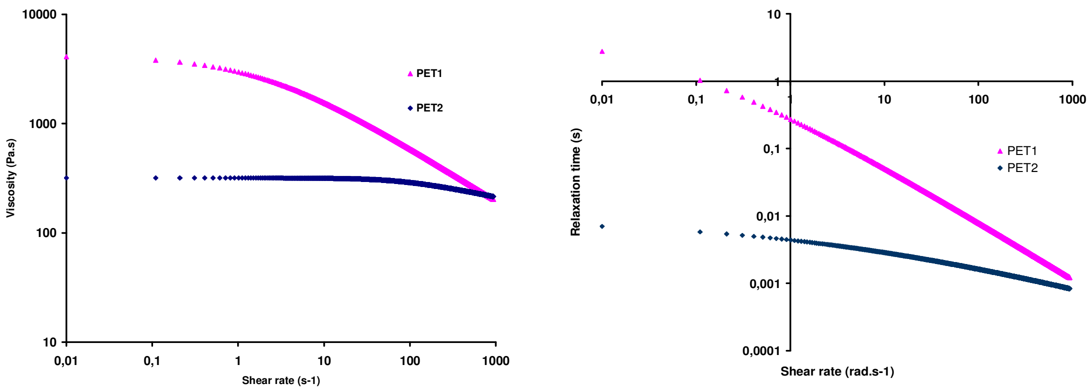


Figure 2 : 1/2 die

View in the thickness direction



A **B**

Figure 3 :Curve of viscosity at 260°C in function of shear rate (A); curve of the relaxation time at 260°C on function of shear rate (B).

Monolayer 3D computation non Isotherm

Coextrusion numerical simulations are carried out using Rem3d® software, developed at Material Forming Centre (CEMEF).

To analyse the flow characteristics inside the die, we performed a 3D calculation of the coat hanger die (with only one layer). We used anisotropic meshing with 55739 nodes and 315314 elements (Figure 4). It enables to have a meshing respectively refined in the thickness and coarse in the two other directions. In the inlet, we impose 46 kg/h flow rate as boundary condition. In the post-processing, we can see the temperature, velocities.

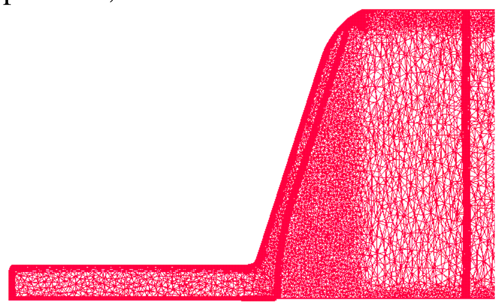


Figure 4 : meshing

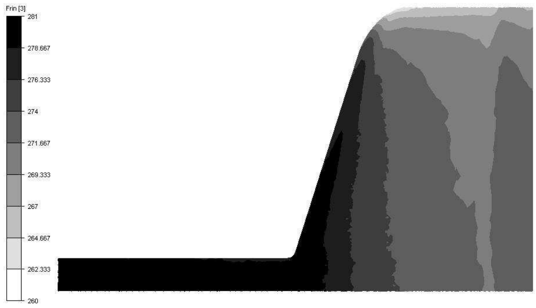


Figure 5 : temperature distribution

This study exhibits the evolution of polymers temperature in the flow direction. Figure 5 illustrated temperature distribution. Inlet temperature polymer is 281°C and the thermal regulation of the die is 260°C. We notice that polymer temperature falls in the flow direction. It decreases mainly after the coat hanger. The exit temperature is 270°C and almost homogeneous at die outlet.

In figure 6, we observe velocity distribution on the flow directions. The higher velocities regions are situated in inlet and outlet zone. We explain this observation by the low width of the inlet and the convergent presence near the outlet. Figure 7 shows velocity distribution in the transverse direction. The velocity is negligible except in the "coat hanger". This fact denotes that the role of the coat hanger is well to bring polymer in the zone furthest away from the feeder canal.

Therefore that the die design of is accurate to distribute the flow of a Newtonian fluid. This is the reason why, we made a dynamic stability 2D analysis both in the feed zone (A) and in the final part of the die (B).

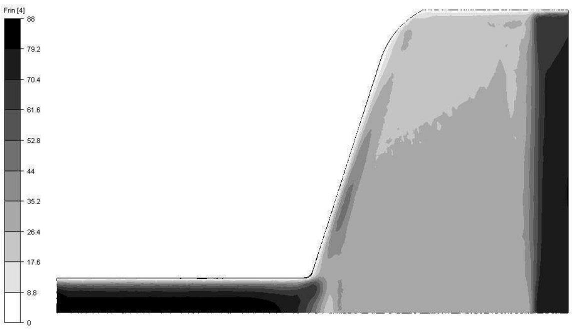


Figure 6 : Velocity In the flow direction

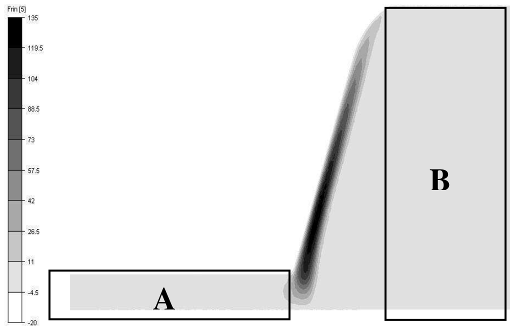


Figure 7 : Velocity In the transverse direction

2D Dynamic stability analysis isothermal

In this part, we analysed successively the A and B zones with two layer calculation. The computational models based purely viscous constitutive equations; with the following law such as:

$$\eta(\dot{\gamma}) = \eta_0 \left[1 + (\lambda\dot{\gamma})^a\right]^{(m-1)/a} \quad (1)$$

Where $\dot{\gamma}$ is the shear rate, η_0 is the zero shear rate viscosity and λ is the relaxation time. Parameter *a* represents the width of the transition region between Newtonian and pseudiplastic, *m* indicates pseudoplastic.

The first calculations isothermal stationary without forcing model allow to determine the position of the interface. To carry out a calculation with forcing, we introduce then a periodic disturbance into the first layer, defined by [8]:

$$Q = Q_0\left(1 + A\sin(\frac{2\pi}{\lambda}t)\right) \quad (2)$$

Where A=0.1, λ forcing period

This disturbance is present in the real case. It comes from a fluctuation of flow precisely related to the screw rotation of the extrusion machine.

The calculation presented in this paper is carried out with a 32kg/h flow rate for PET1 and 80 kg/h for PET2. In Figure 8, we can see interface position.

Figure 8 : Stationary solution in the feed zone

To analyse the interface, we implemented an interface position calculation from the finite elements solution. From this result we can make analyse space-time.

The space-time analyses (Figures 9 and 10) with a forcing frequency of 3.6 Hz show a space and temporal periodicity of the disturbance. Indeed, the disturbance generates defects in progressives waves form. These instability magnitudes decreased gradually when we get closer to the die exit.

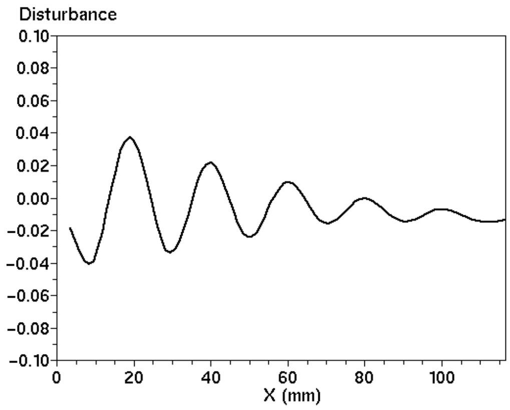


Figure 9 : Relative variation of disturbance as a function of die length, frequency forcing: 3.6Hz

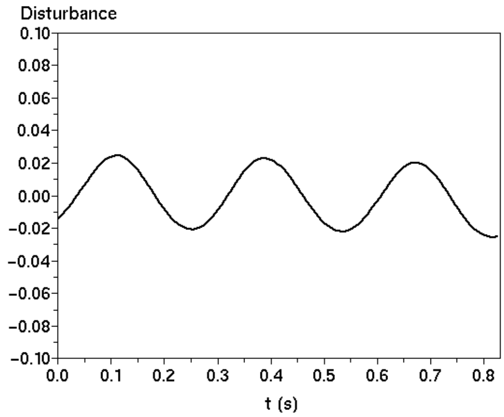


Figure 10 : Relative variation of disturbance as a function of time

We analysed then zone B. In the post-process, we observe interface position (Figure 11). We want to know convergent influence on the disturbances.

Figure 11 : Stationary solution in the final part of the die.

In this case, the disturbance generates defects in progressives waves form as we observed previously for feed die calculations. These instability magnitudes decreased gradually when we get closer to the die exit but the magnitudes is less important than in the feed zone (Figure 12).

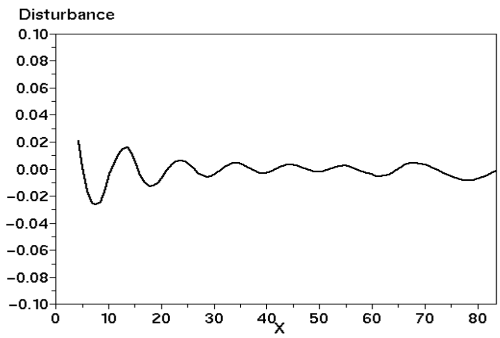


Figure 12 : Relative variation of disturbance as a function of die length, frequency forcing: 3.6Hz

2D Dynamic stability analysis non-isothermal

Industry uses temperature variation to stabilise the instabilities in interfaces. This part deals with about the impact of polymers and die temperatures. Polymers rheologies are thermo dependant, following Arrhenius law. In Figure 13, we observe the comparison between isothermal and non isothermal computations. For non-isothermal case; polymers temperatures are 281°C for PET1 and 255°C for PET2. The thermal regulation of the die is 260°C. For non isothermal calculations, that thermal parameters, which modify the rheology of both polymers, have a significative influence on the disturbance amplitude.

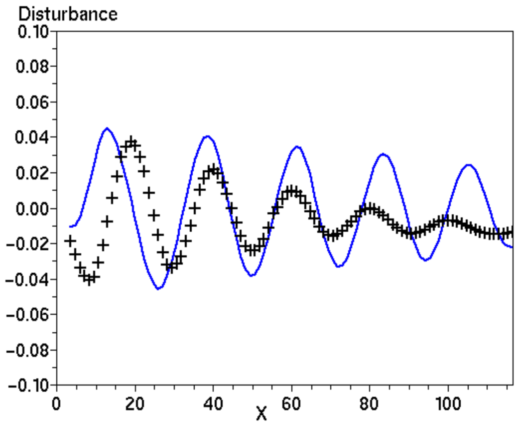


Figure 13 : comparison of relative variation of disturbance as a function of time between isotherm (-) and non isotherm (+).

These results have been obtained by using purely viscous constitutive equations. With this model, we use Reynolds number as instabilities motor, but this value is very low. Now, we are developing viscoelastic computation with multi-Maxwell model where the motor of instability is the number of Weissenberg. This number can take considerable values.

CONCLUSION

A 3D calculation of the coat hanger dire (with only one layer) points out that the flow is one-dimensional except for the "coat hanger" part. That why we perform a 2D dynamic stability analysis both in the feed zone of the die and in the final part of the die. For given flows and frequencies, the introduced disturbance generates defects in progressives waves form. These instability amplitudes decreased gradually when it gets closer to the die exit whatsoever the zone study. Non isothermal calculations point out that thermal parameters have an influence on the disturbance amplitude.

The first viscoelastic calculation showed that the instability magnitude increases when we get closer to the die exit, contrary to purely viscous calculations. Those results are en agreement to the ones found in the literature [1].

ACKNOWLEDGMENTS

The authors would like to thank F. Fournier from centre for Material Forming (CEMEF) and S. Freville from Arcelor packaging.

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